

Tris(2-chloroisopropyl)phosphate
13674-84-5 | DTXSID5026259

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.68e-03 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.48e-01

Confidence level: 3.69e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Linalyl acetate</div> <div>Measured: 6.13e-02</div> <div>Predicted: 8.66e-02</div>	<div>Image not found</div> <div>1-Nonene</div> <div>Measured: 1.13e-03</div> <div>Predicted: 7.39</div>	<div>Image not found</div> <div>Bendiocarb</div> <div>Measured: 1.28e-03</div> <div>Predicted: 1.68e-05</div>
<div>Image not found</div> <div>4-Thiocresol</div> <div>Measured: 1.48e-03</div> <div>Predicted: 7.46e-01</div>	<div>Image not found</div> <div>Pyrimethanil</div> <div>Measured: 7.95e-04</div> <div>Predicted: 2.40e-06</div>	